wwPDB EM Validation Summary Report

Nov 20, 2022 – 04:04 pm GMT

PDB ID	:	2YKR
EMDB ID	:	EMD-1884
Title	:	30S ribosomal subunit with RsgA bound in the presence of GMPPNP
Authors	:	Guo, Q.; Yuan, Y.; Xu, Y.; Feng, B.; Liu, L.; Chen, K.; Lei, J.; Gao, N.
Deposited on	:	2011-05-30
Resolution	:	9.80 Å(reported)
Based on initial models	:	2RCN, 3OFA

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

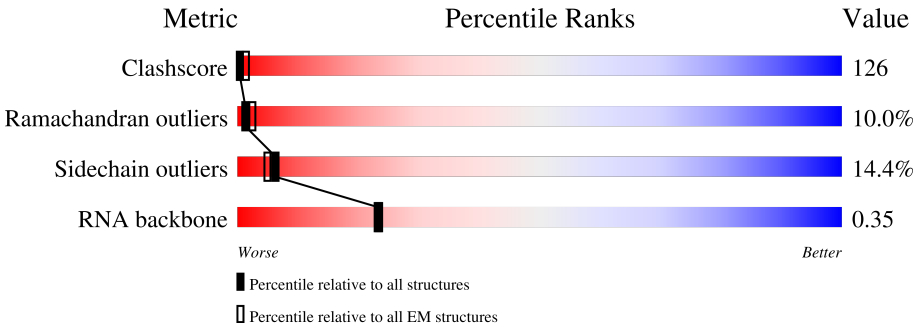
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 9.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1533	14% 86%
2	B	218	26% 44% 24% 6%
3	C	206	27% 43% 25% 5%
4	D	205	29% 48% 16% 7%
5	E	150	21% 51% 19% 9%
6	F	100	31% 40% 21% 8%
7	G	151	9% 52% 32% 11% 5%

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Mol	Chain	Length	Quality of chain
8	H	129	26% 39% 26% 9%
9	I	127	31% 41% 17% 12%
10	J	98	21% 50% 18% 10%
11	K	117	30% 37% 28% 5%
12	L	123	33% 41% 18% 9%
13	M	114	25% 35% 26% 13%
14	N	100	29% 40% 20% 8%
15	O	88	25% 47% 20% 8%
16	P	82	28% 43% 23% 6%
17	Q	80	18% 32% 36% 14%
18	R	55	29% 49% 16% 5%
19	S	79	32% 43% 16% 9%
20	T	85	31% 44% 21% 5%
21	U	51	37% 57% 33% 6%
22	W	350	38% 30% 11% 19%

2 Entry composition (i)

There are 22 unique types of molecules in this entry. The entry contains 53633 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	1533	32892	14671	6036	10653	1532	0	0

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	218	1705	1081	305	312	7	0	0

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	206	1625	1028	305	289	3	0	0

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	205	1643	1026	315	298	4	0	0

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	150	1106	687	211	202	6	0	0

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	100	818	515	148	149	6	0	0

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	151	Total	C	N	O	S	0	0
			1182	735	227	216	4		

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	98	Total	C	N	O	S	0	0
			787	493	150	143	1		

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	114	Total	C	N	O	S	0	0
			884	546	178	157	3		

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	97	Total	C	N	O	S	0	1
			775	483	161	128	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	39	ASP	GLU	conflict	UNP B7M1M1

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	80	Total	C	N	O	S	0	0
			649	411	121	114	3		

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	R	55	Total	C	N	O	0	0
			456	288	86	82		

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	79	Total	C	N	O	S	0	0
			638	408	120	108	2		

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	51	Total	C	N	O	S	0	0
			426	265	86	74	1		

- Molecule 22 is a protein called PUTATIVE RIBOSOME BIOGENESIS GTPASE RSGA.

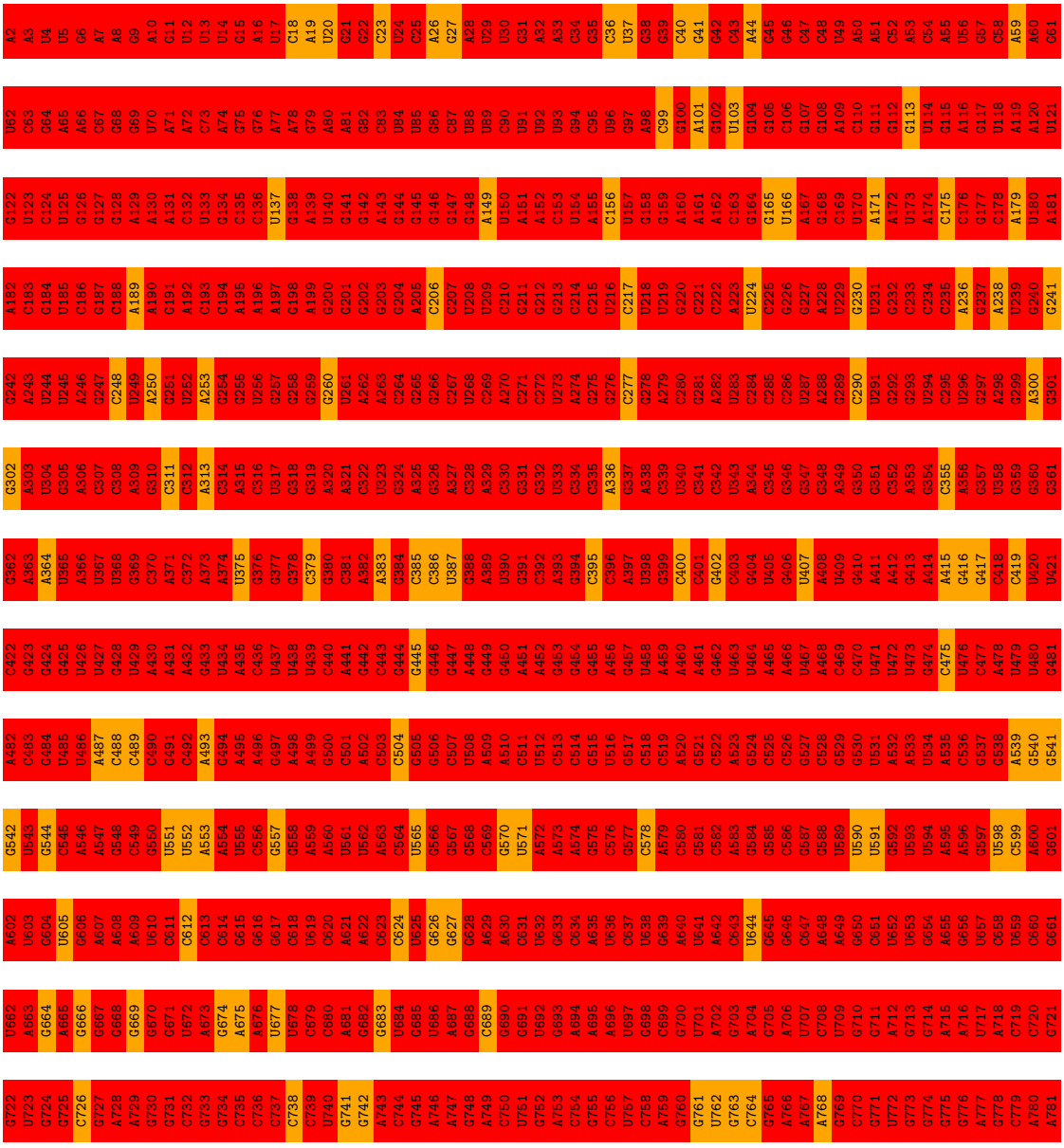
Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	282	Total	C	N	O	S	0	4
			2186	1378	388	410	10		

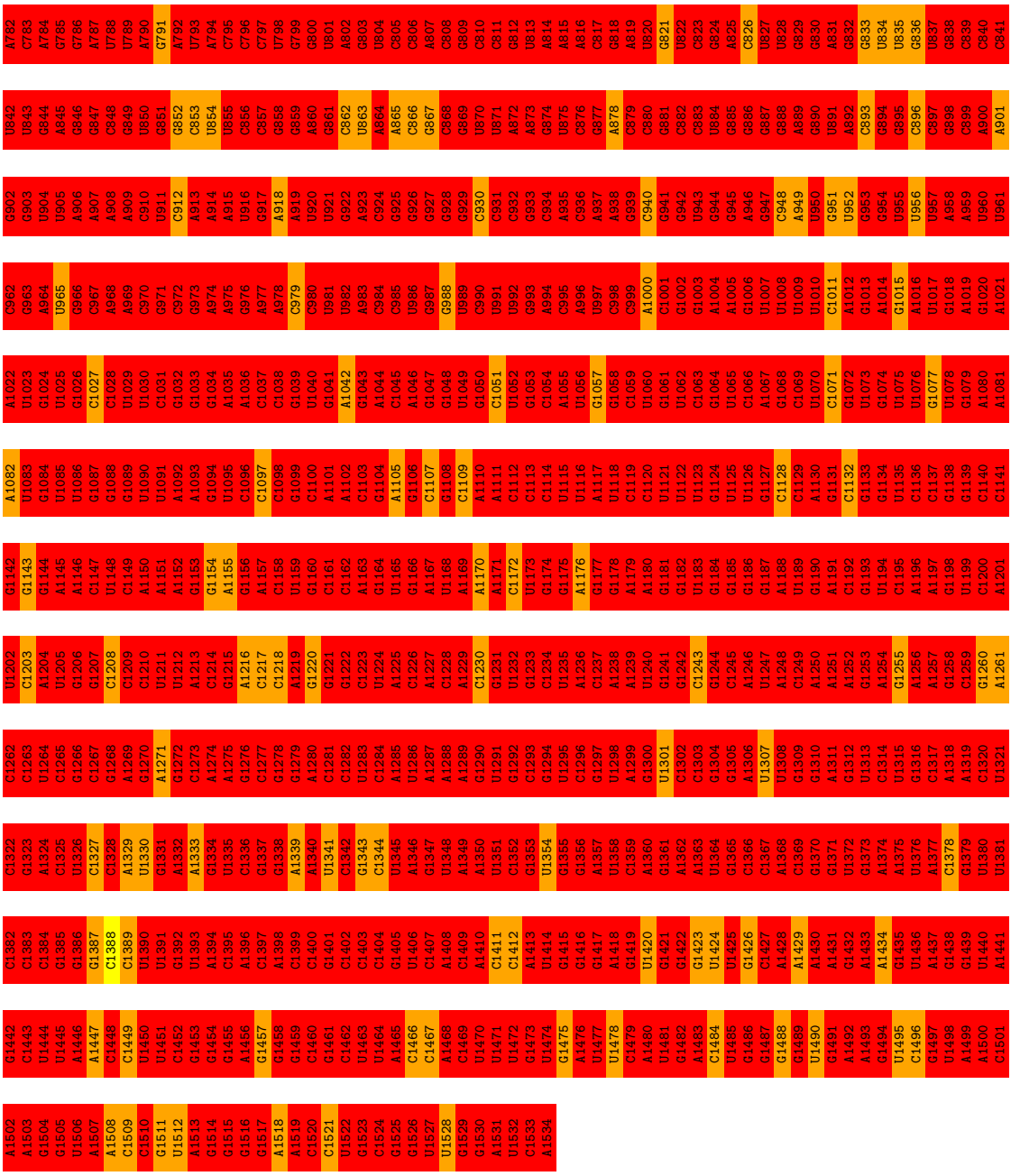
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 16S RRNA

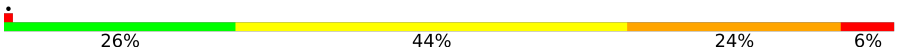
Chain A:

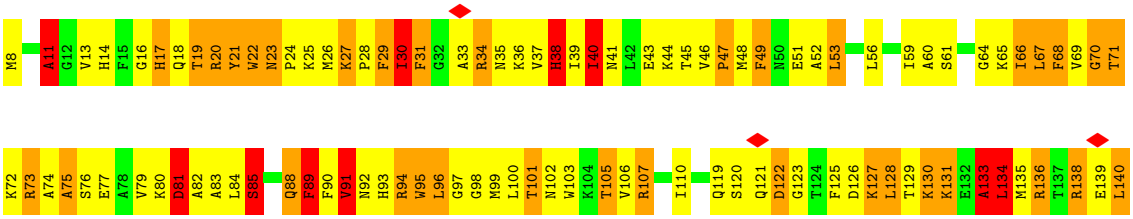


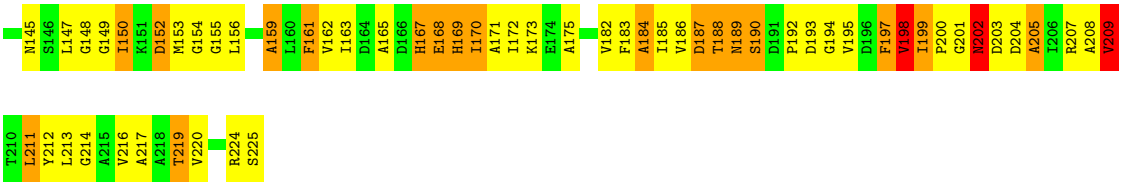


• Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain B:

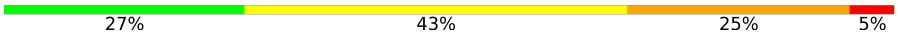


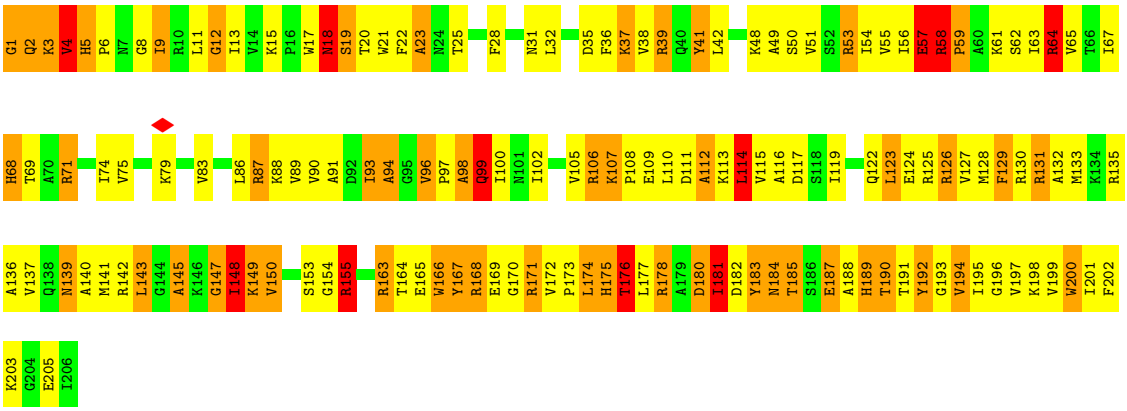




• Molecule 3: 30S RIBOSOMAL PROTEIN S3

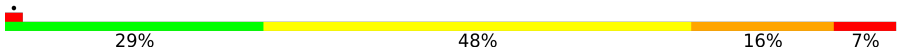
Chain C:

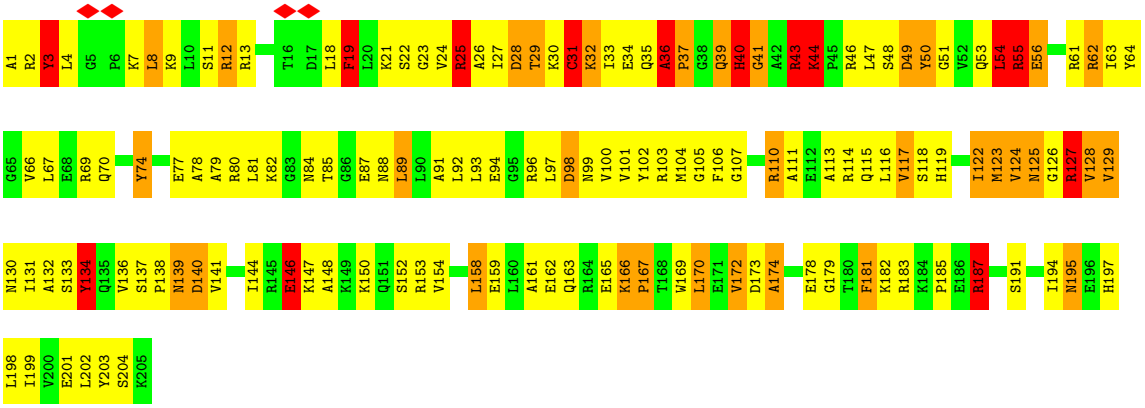




• Molecule 4: 30S RIBOSOMAL PROTEIN S4

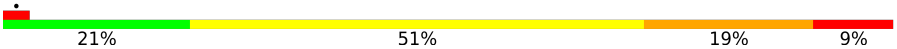
Chain D:

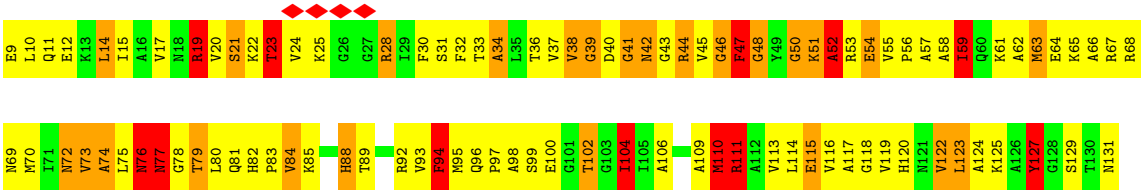




• Molecule 5: 30S RIBOSOMAL PROTEIN S5

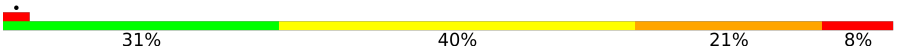
Chain E:

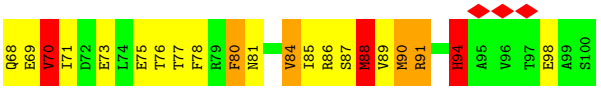




• Molecule 6: 30S RIBOSOMAL PROTEIN S6

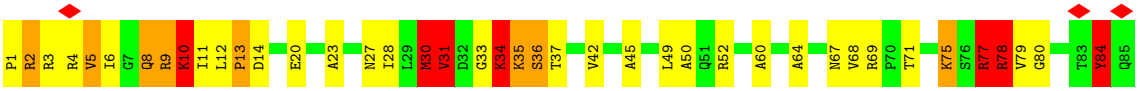
Chain F:

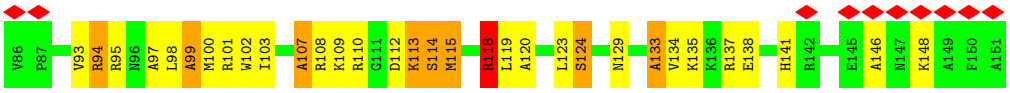




• Molecule 7: 30S RIBOSOMAL PROTEIN S7

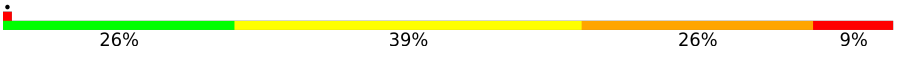
Chain G:

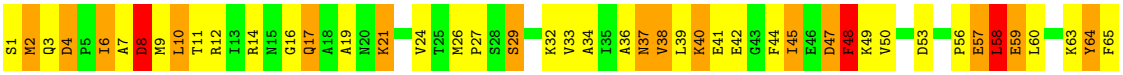


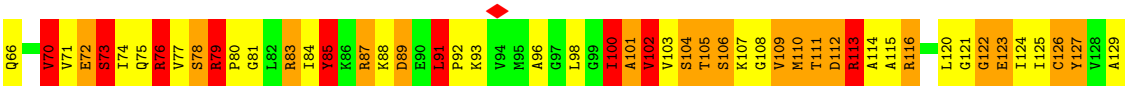


• Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain H:

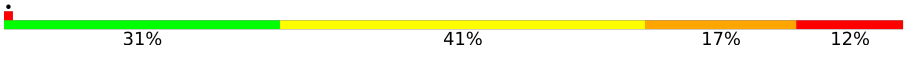


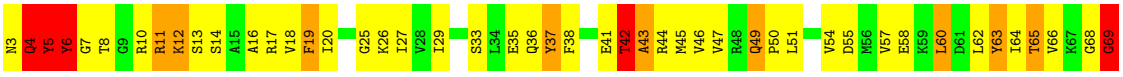


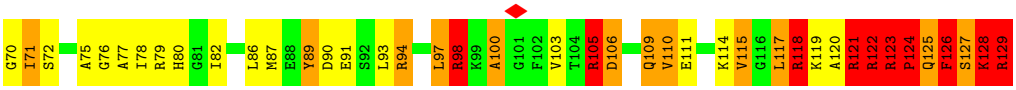


• Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain I:

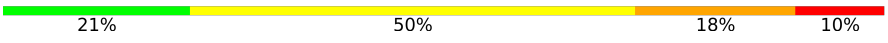


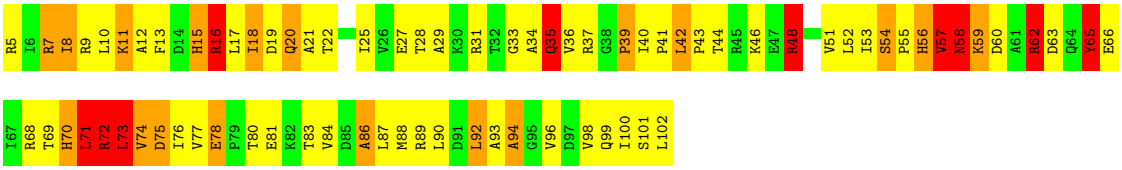




• Molecule 10: 30S RIBOSOMAL PROTEIN S10

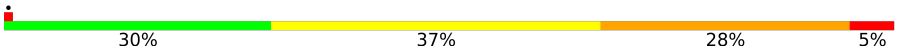
Chain J:

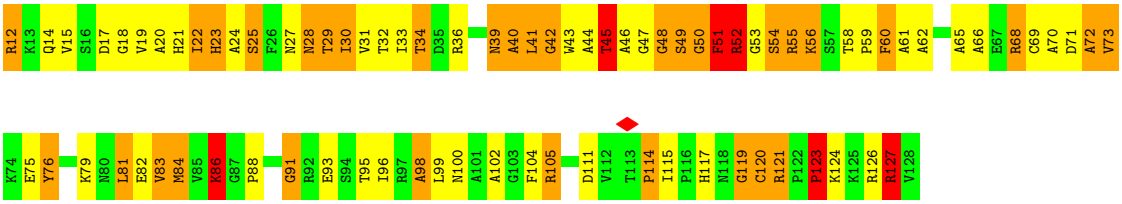




• Molecule 11: 30S RIBOSOMAL PROTEIN S11

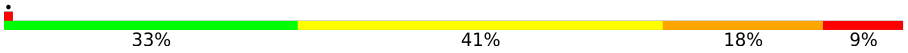
Chain K:

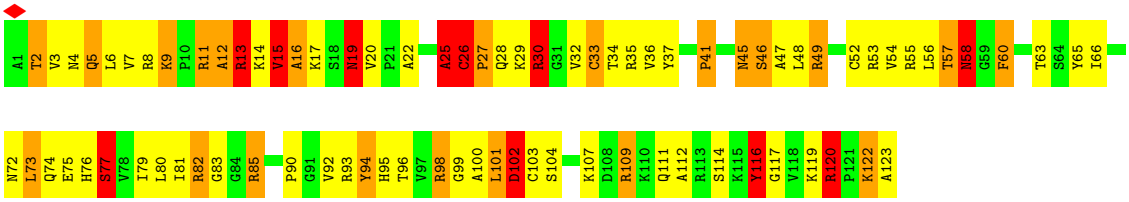




• Molecule 12: 30S RIBOSOMAL PROTEIN S12

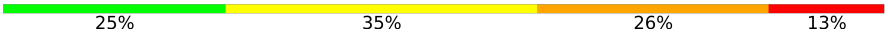
Chain L:

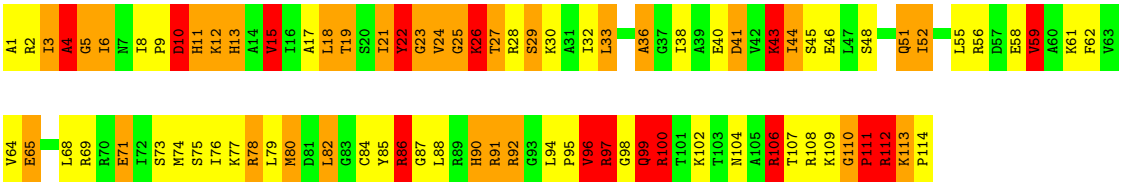




• Molecule 13: 30S RIBOSOMAL PROTEIN S13

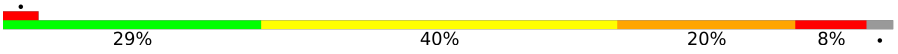
Chain M:

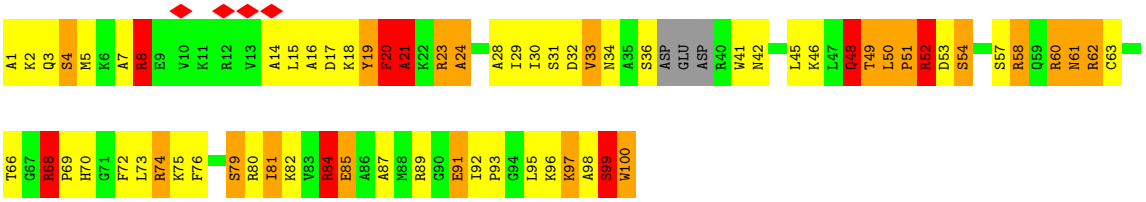




• Molecule 14: 30S RIBOSOMAL PROTEIN S14

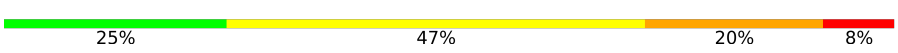
Chain N:

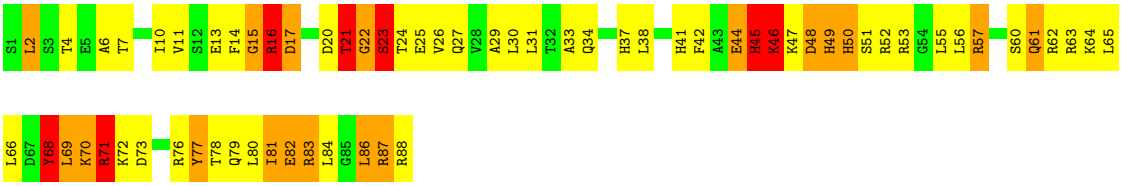




• Molecule 15: 30S RIBOSOMAL PROTEIN S15

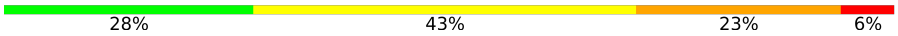
Chain O:

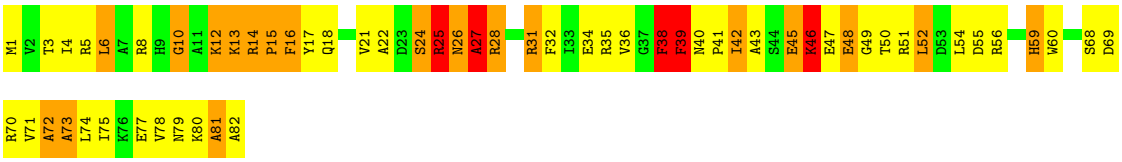




• Molecule 16: 30S RIBOSOMAL PROTEIN S16

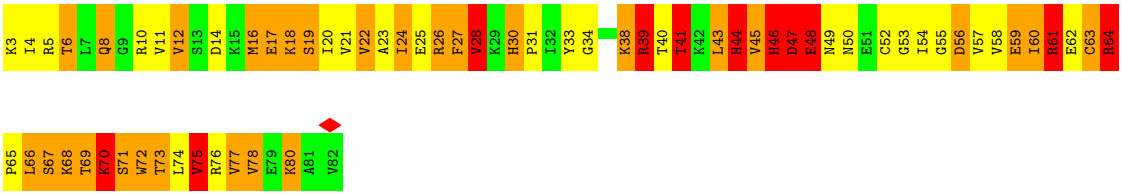
Chain P:





• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain Q:

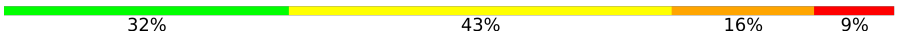


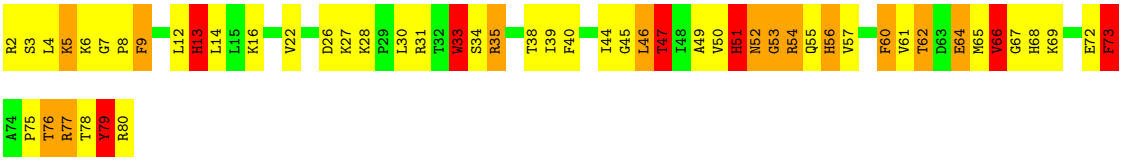
• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain R:

• Molecule 19: 30S RIBOSOMAL PROTEIN S19

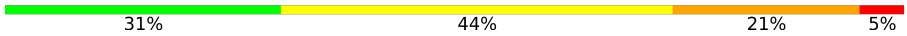
Chain S:

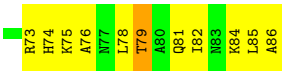




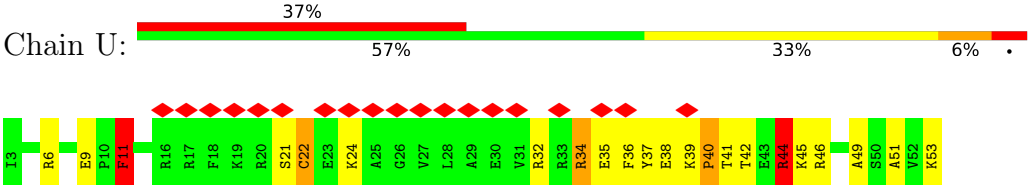
• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain T:

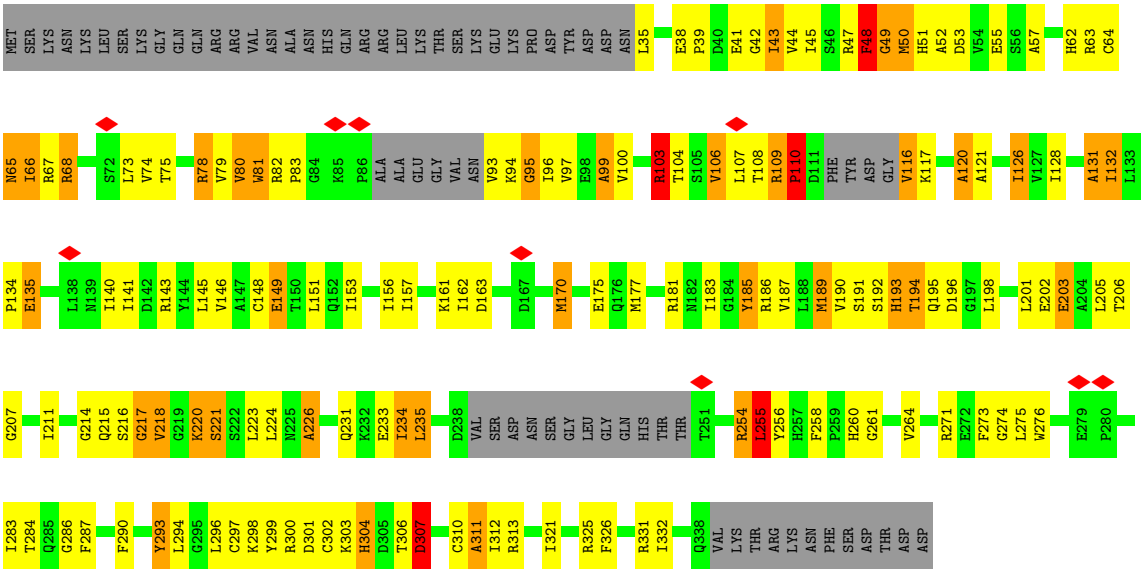




• Molecule 21: 30S RIBOSOMAL PROTEIN S21



• Molecule 22: PUTATIVE RIBOSOME BIOGENESIS GTPASE RSGA



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	77483	Depositor
Resolution determination method	Not provided	
CTF correction method	MAPS FROM EACH DEFOCUS GROUP	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3850	Depositor
Magnification	59000	Depositor
Image detector	FEI EAGLE (4k x 4k)	Depositor
Maximum map value	19.771	Depositor
Minimum map value	-6.451	Depositor
Average map value	0.106	Depositor
Map value standard deviation	1.371	Depositor
Recommended contour level	3.16	Depositor
Map size (Å)	362.5, 362.5, 362.5	wwPDB
Map dimensions	125, 125, 125	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	2.9, 2.9, 2.9	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	3.88	6344/36831 (17.2%)	4.27	11020/57458 (19.2%)
2	B	1.35	2/1736 (0.1%)	1.90	59/2338 (2.5%)
3	C	1.48	2/1652 (0.1%)	1.88	48/2225 (2.2%)
4	D	1.45	4/1665 (0.2%)	1.82	40/2227 (1.8%)
5	E	1.57	8/1119 (0.7%)	1.93	38/1504 (2.5%)
6	F	1.37	1/836 (0.1%)	1.96	29/1128 (2.6%)
7	G	1.27	2/1196 (0.2%)	1.59	18/1602 (1.1%)
8	H	1.42	2/989 (0.2%)	1.96	36/1326 (2.7%)
9	I	1.45	1/1034 (0.1%)	1.93	36/1375 (2.6%)
10	J	1.41	0/797	2.00	23/1077 (2.1%)
11	K	1.61	4/893 (0.4%)	1.82	24/1205 (2.0%)
12	L	1.42	1/969 (0.1%)	1.88	27/1300 (2.1%)
13	M	1.60	5/893 (0.6%)	1.97	30/1193 (2.5%)
14	N	1.33	0/786	1.93	19/1045 (1.8%)
15	O	1.42	2/722 (0.3%)	1.99	26/964 (2.7%)
16	P	1.42	0/659	2.00	27/884 (3.1%)
17	Q	1.69	4/658 (0.6%)	2.31	40/881 (4.5%)
18	R	1.35	0/463	1.99	14/621 (2.3%)
19	S	1.20	1/653 (0.2%)	1.69	14/877 (1.6%)
20	T	1.37	1/671 (0.1%)	1.96	18/888 (2.0%)
21	U	1.28	0/431	1.60	2/570 (0.4%)
22	W	1.30	3/2223 (0.1%)	1.58	40/3008 (1.3%)
All	All	3.21	6387/57876 (11.0%)	3.66	11628/85696 (13.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1238
2	B	0	14
3	C	0	16

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	15
5	E	0	6
6	F	0	7
7	G	0	4
8	H	0	12
9	I	0	15
10	J	0	6
11	K	0	10
12	L	0	7
13	M	0	13
14	N	0	9
15	O	0	9
16	P	0	5
17	Q	0	7
18	R	0	4
19	S	0	8
20	T	0	5
21	U	0	2
22	W	0	7
All	All	0	1419

The worst 5 of 6387 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1306	A	N7-C5	-22.89	1.25	1.39
1	A	466	A	N7-C5	-22.87	1.25	1.39
1	A	627	G	N7-C5	-22.74	1.25	1.39
1	A	373	A	N9-C4	-22.28	1.24	1.37
1	A	78	A	N9-C4	22.19	1.51	1.37

The worst 5 of 11628 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1399	C	P-O3'-C3'	47.06	176.18	119.70
1	A	1139	G	P-O3'-C3'	47.02	176.13	119.70
1	A	556	C	C6-N1-C2	-44.83	102.37	120.30
1	A	306	A	P-O3'-C3'	39.05	166.56	119.70
1	A	73	C	C6-N1-C2	-38.49	104.91	120.30

There are no chirality outliers.

5 of 1419 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	A	Sidechain
1	A	3	A	Sidechain
1	A	4	U	Sidechain
1	A	5	U	Sidechain
1	A	6	G	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32892	0	16464	9848	0
2	B	1705	0	1732	204	0
3	C	1625	0	1699	204	0
4	D	1643	0	1710	176	0
5	E	1106	0	1148	142	0
6	F	818	0	808	110	0
7	G	1182	0	1239	124	0
8	H	979	0	1034	139	0
9	I	1022	0	1070	132	0
10	J	787	0	828	130	0
11	K	877	0	887	165	0
12	L	955	0	1019	106	0
13	M	884	0	944	126	0
14	N	775	0	827	111	0
15	O	714	0	737	111	0
16	P	649	0	666	67	0
17	Q	649	0	690	143	0
18	R	456	0	478	57	0
19	S	638	0	665	75	0
20	T	665	0	714	109	0
21	U	426	0	449	19	0
22	W	2186	0	2180	107	0
All	All	53633	0	37988	11504	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 126.

The worst 5 of 11504 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:U:H5'	4:D:8:LEU:HD13	1.45	0.99
1:A:688:G:H5"	1:A:688:G:C8	1.99	0.98
1:A:82:G:H22	1:A:84:U:H3	1.11	0.95
1:A:450:G:H1	1:A:483:C:H42	1.13	0.95
1:A:1469:C:H5'	1:A:1469:C:C6	2.02	0.94

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	216/218 (99%)	149 (69%)	41 (19%)	26 (12%)	0 6
3	C	204/206 (99%)	158 (78%)	28 (14%)	18 (9%)	1 11
4	D	203/205 (99%)	139 (68%)	41 (20%)	23 (11%)	0 7
5	E	148/150 (99%)	104 (70%)	25 (17%)	19 (13%)	0 5
6	F	98/100 (98%)	75 (76%)	16 (16%)	7 (7%)	1 14
7	G	149/151 (99%)	118 (79%)	20 (13%)	11 (7%)	1 14
8	H	127/129 (98%)	90 (71%)	26 (20%)	11 (9%)	1 11
9	I	125/127 (98%)	83 (66%)	25 (20%)	17 (14%)	0 4
10	J	96/98 (98%)	74 (77%)	10 (10%)	12 (12%)	0 5
11	K	115/117 (98%)	81 (70%)	20 (17%)	14 (12%)	0 6
12	L	121/123 (98%)	85 (70%)	22 (18%)	14 (12%)	0 6
13	M	112/114 (98%)	82 (73%)	16 (14%)	14 (12%)	0 5
14	N	93/100 (93%)	61 (66%)	21 (23%)	11 (12%)	0 6
15	O	86/88 (98%)	65 (76%)	16 (19%)	5 (6%)	1 18
16	P	80/82 (98%)	58 (72%)	13 (16%)	9 (11%)	0 7
17	Q	78/80 (98%)	55 (70%)	16 (20%)	7 (9%)	1 11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
18	R	53/55 (96%)	33 (62%)	12 (23%)	8 (15%)	0 3
19	S	77/79 (98%)	61 (79%)	12 (16%)	4 (5%)	2 19
20	T	83/85 (98%)	64 (77%)	14 (17%)	5 (6%)	1 17
21	U	49/51 (96%)	28 (57%)	11 (22%)	10 (20%)	0 2
22	W	274/350 (78%)	236 (86%)	25 (9%)	13 (5%)	2 21
All	All	2587/2708 (96%)	1899 (73%)	430 (17%)	258 (10%)	1 9

5 of 258 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	11	ALA
2	B	18	GLN
2	B	23	ASN
2	B	27	LYS
2	B	30	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	180/180 (100%)	156 (87%)	24 (13%)	4 18
3	C	170/170 (100%)	146 (86%)	24 (14%)	3 16
4	D	172/172 (100%)	147 (86%)	25 (14%)	3 15
5	E	113/113 (100%)	94 (83%)	19 (17%)	2 12
6	F	87/87 (100%)	74 (85%)	13 (15%)	3 15
7	G	124/124 (100%)	113 (91%)	11 (9%)	9 30
8	H	104/104 (100%)	84 (81%)	20 (19%)	1 8
9	I	105/105 (100%)	91 (87%)	14 (13%)	4 18
10	J	86/86 (100%)	71 (83%)	15 (17%)	2 11
11	K	90/90 (100%)	75 (83%)	15 (17%)	2 12
12	L	103/103 (100%)	88 (85%)	15 (15%)	3 15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
13	M	92/92 (100%)	74 (80%)	18 (20%)	1 8
14	N	79/83 (95%)	67 (85%)	12 (15%)	3 14
15	O	76/76 (100%)	68 (90%)	8 (10%)	7 24
16	P	65/65 (100%)	57 (88%)	8 (12%)	4 19
17	Q	74/74 (100%)	52 (70%)	22 (30%)	0 2
18	R	48/48 (100%)	44 (92%)	4 (8%)	11 34
19	S	70/70 (100%)	58 (83%)	12 (17%)	2 11
20	T	65/65 (100%)	56 (86%)	9 (14%)	3 17
21	U	44/44 (100%)	40 (91%)	4 (9%)	9 29
22	W	238/302 (79%)	215 (90%)	23 (10%)	8 27
All	All	2185/2253 (97%)	1870 (86%)	315 (14%)	6 16

5 of 315 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	O	79	GLN
20	T	69	ASN
16	P	59	HIS
17	Q	70	LYS
22	W	116	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
11	K	28	ASN
15	O	49	HIS
22	W	215	GLN
11	K	117	HIS
14	N	70	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1532/1533 (99%)	479 (31%)	200 (13%)

5 of 479 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	3	A
1	A	4	U
1	A	5	U
1	A	6	G
1	A	7	A

5 of 200 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	817	C
1	A	1087	G
1	A	1533	C
1	A	845	A
1	A	974	A

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	70:U	O3'	71:A	P	1.39

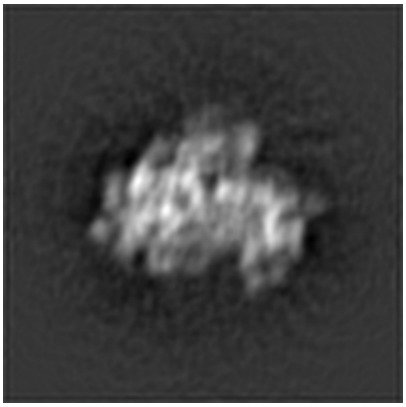
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-1884. These allow visual inspection of the internal detail of the map and identification of artifacts.

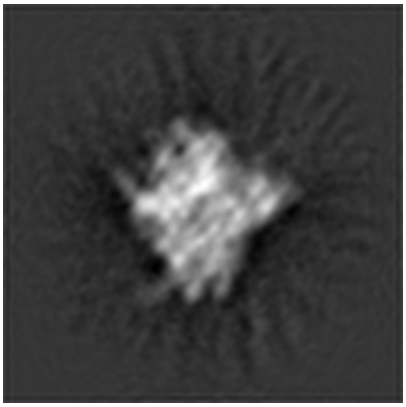
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

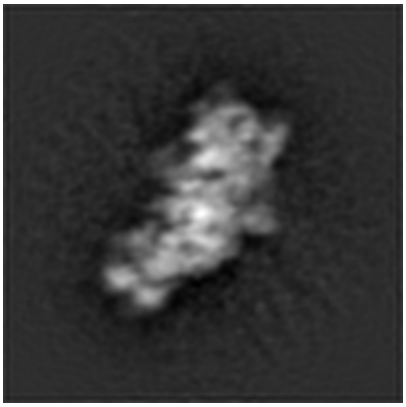
6.1.1 Primary map



X



Y

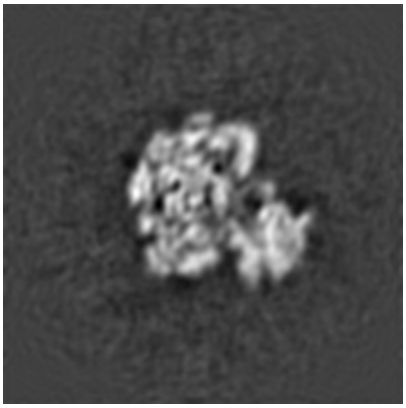


Z

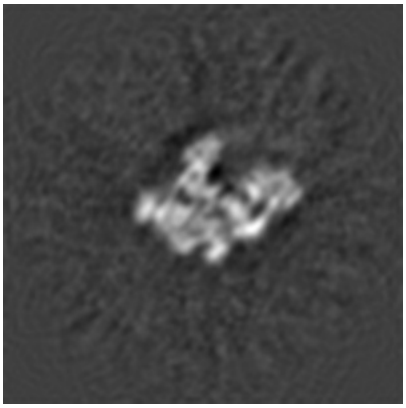
The images above show the map projected in three orthogonal directions.

6.2 Central slices

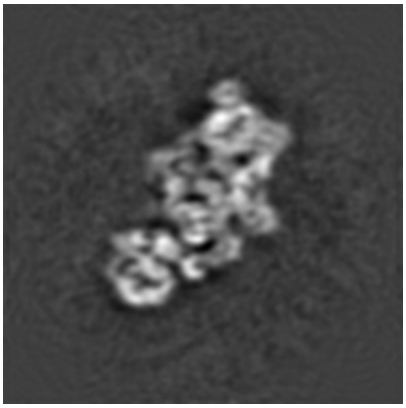
6.2.1 Primary map



X Index: 62



Y Index: 62

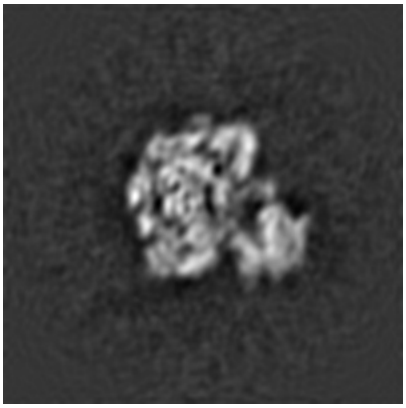


Z Index: 62

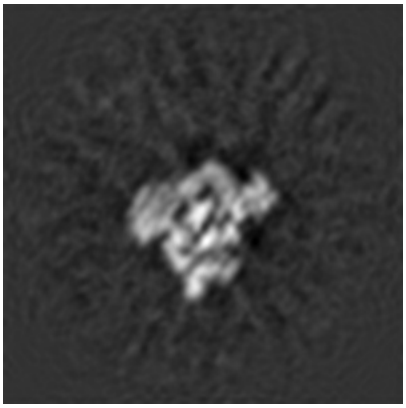
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

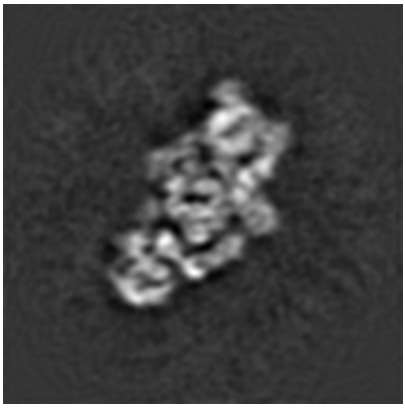
6.3.1 Primary map



X Index: 61



Y Index: 51

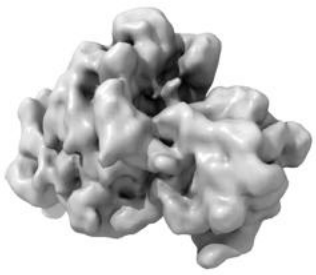


Z Index: 63

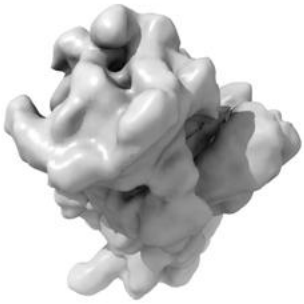
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

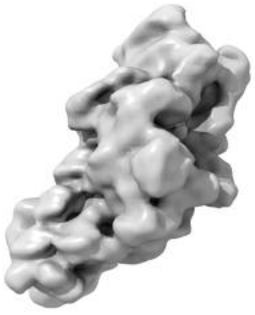
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.16. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

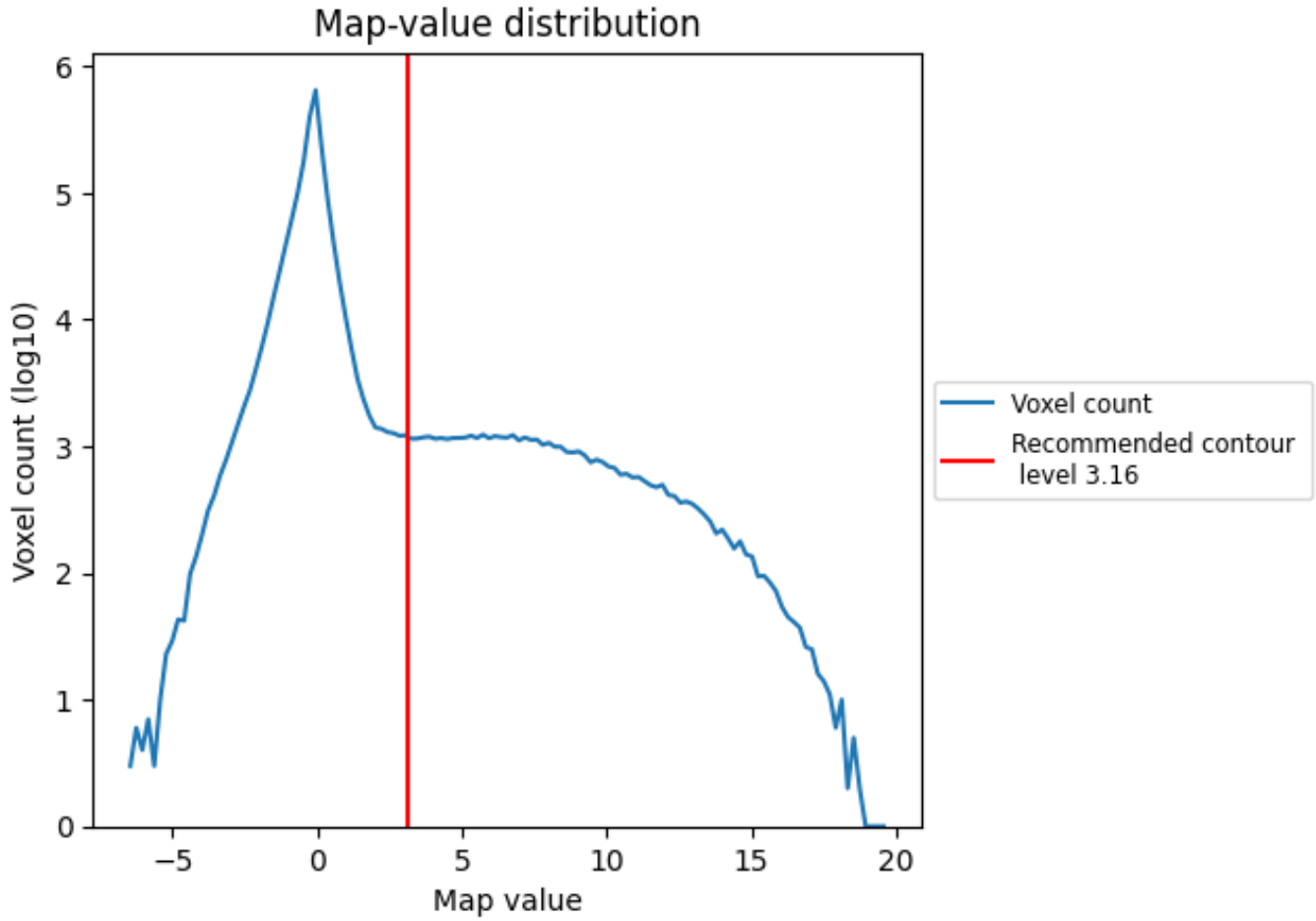
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

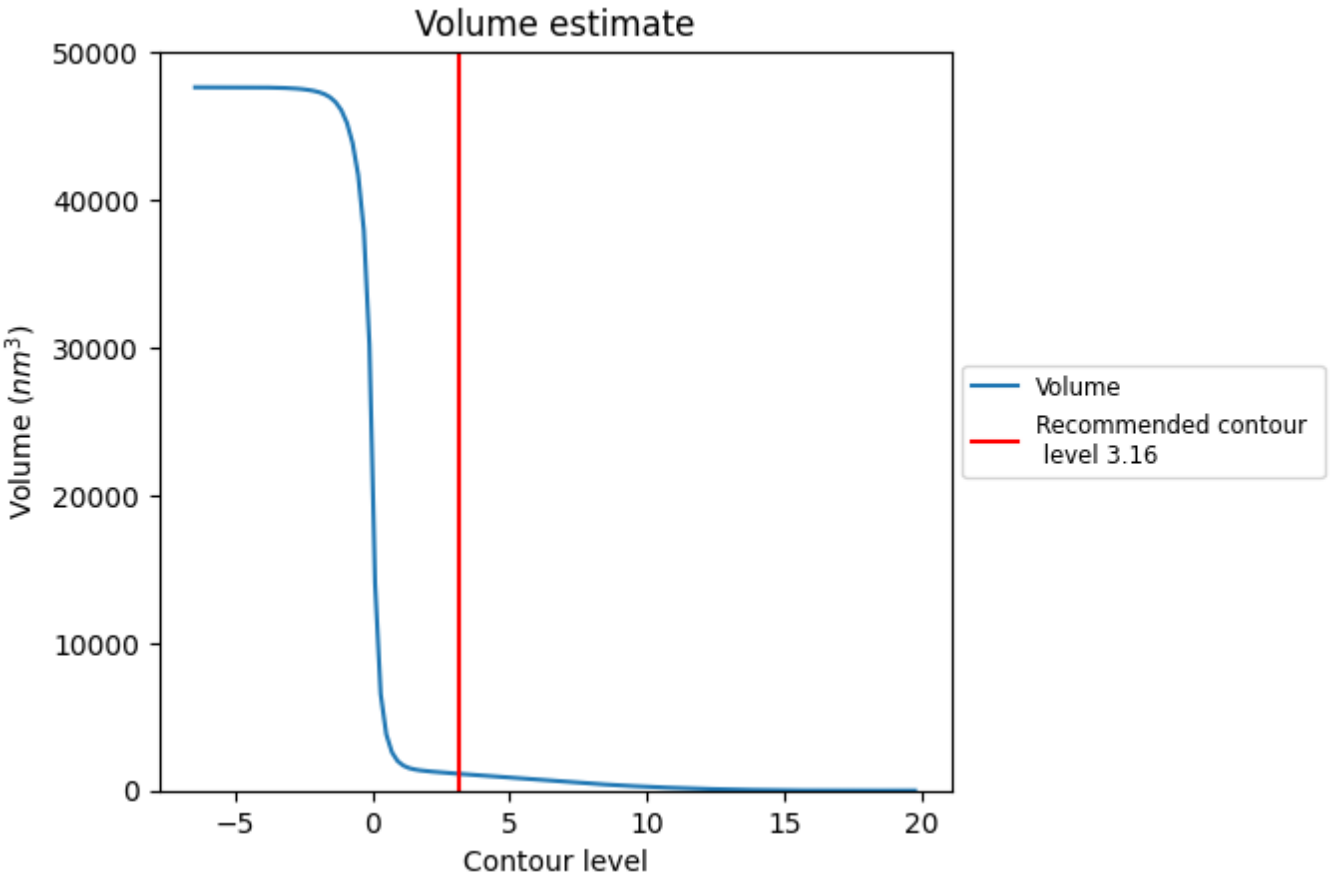
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

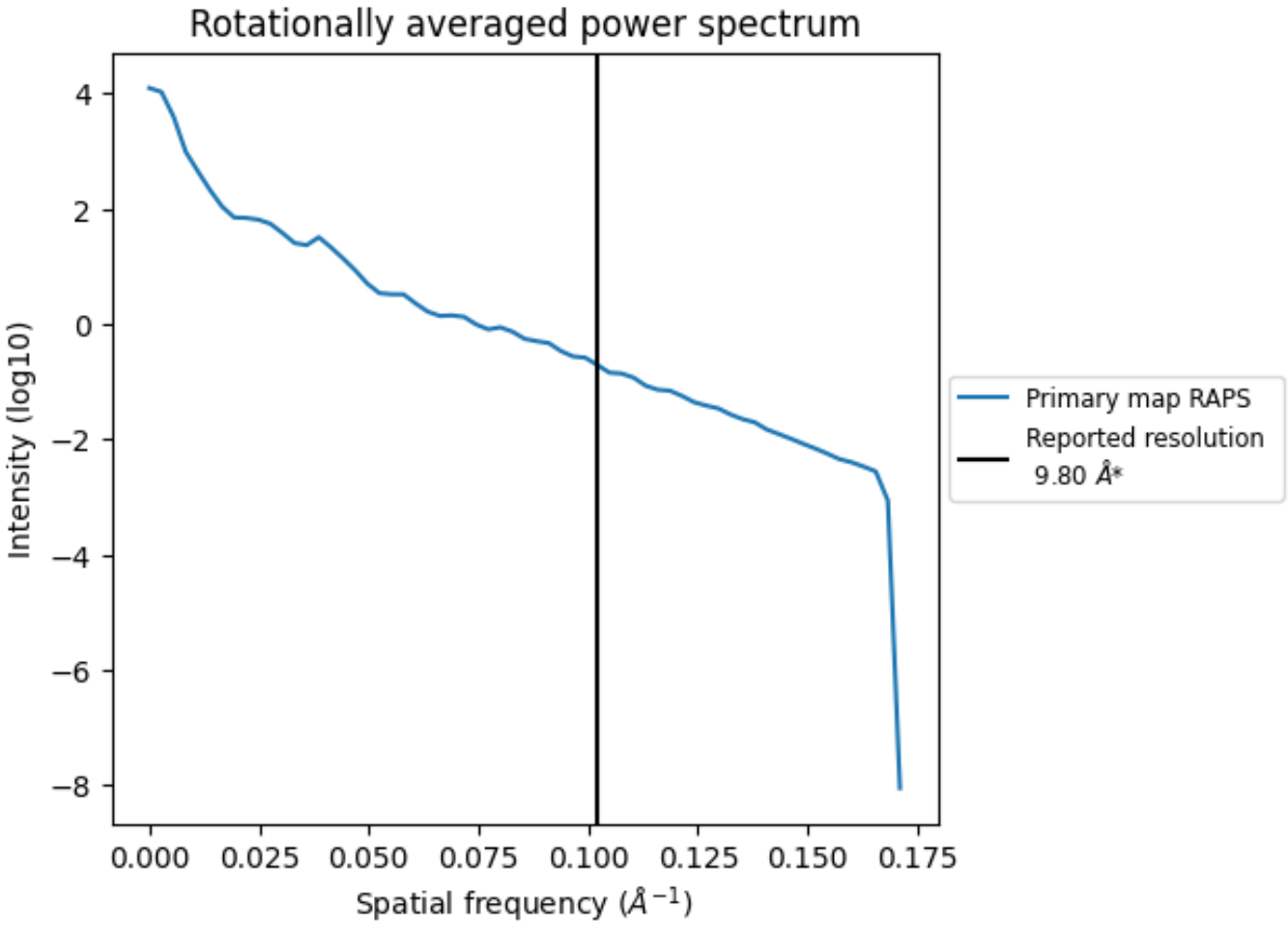
7.2 Volume estimate (i)



The volume at the recommended contour level is 1134 nm^3; this corresponds to an approximate mass of 1025 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.102 Å^{-1}

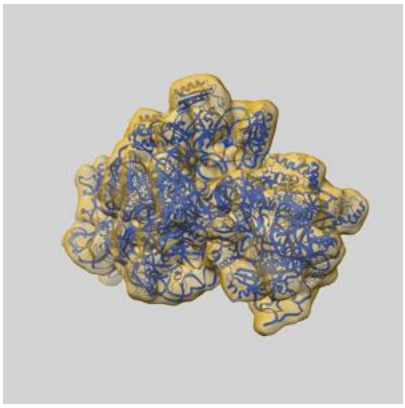
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

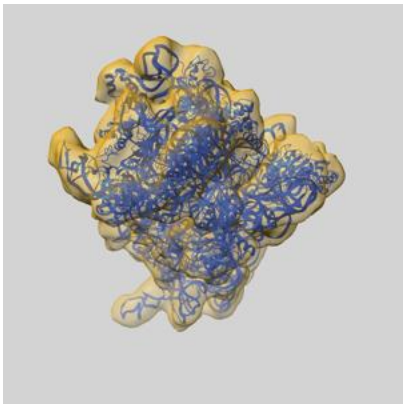
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-1884 and PDB model 2YKR. Per-residue inclusion information can be found in section 3 on page 8.

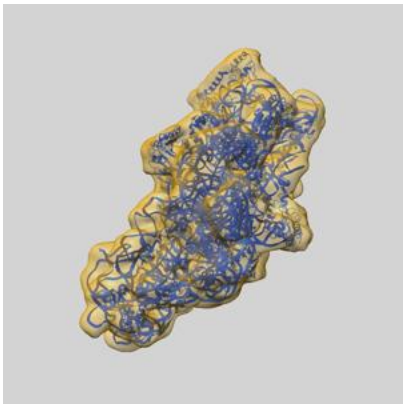
9.1 Map-model overlay



X



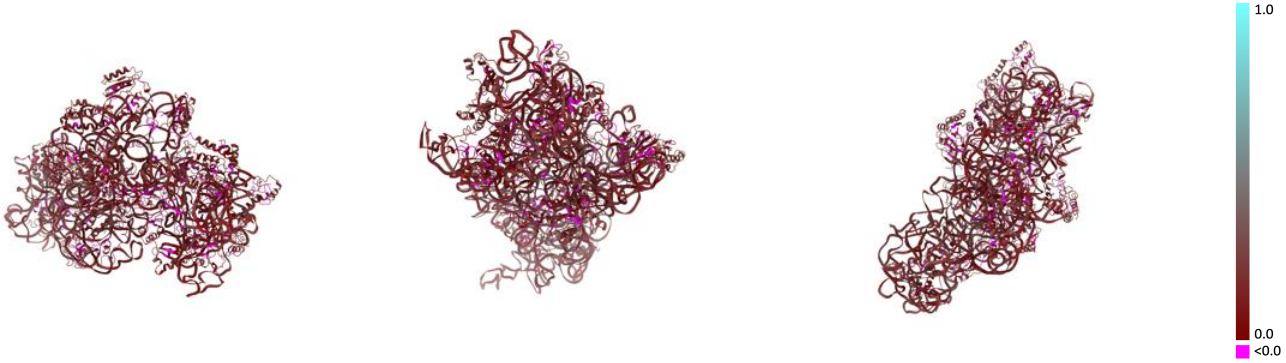
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

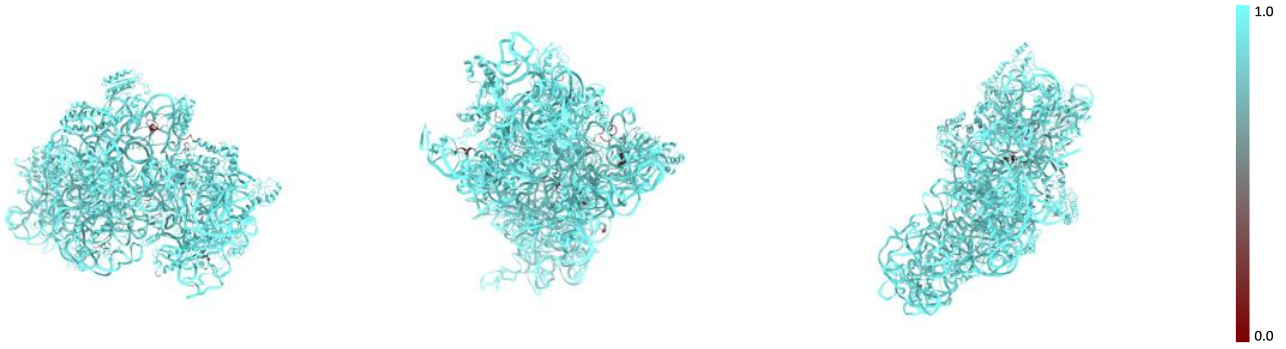
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

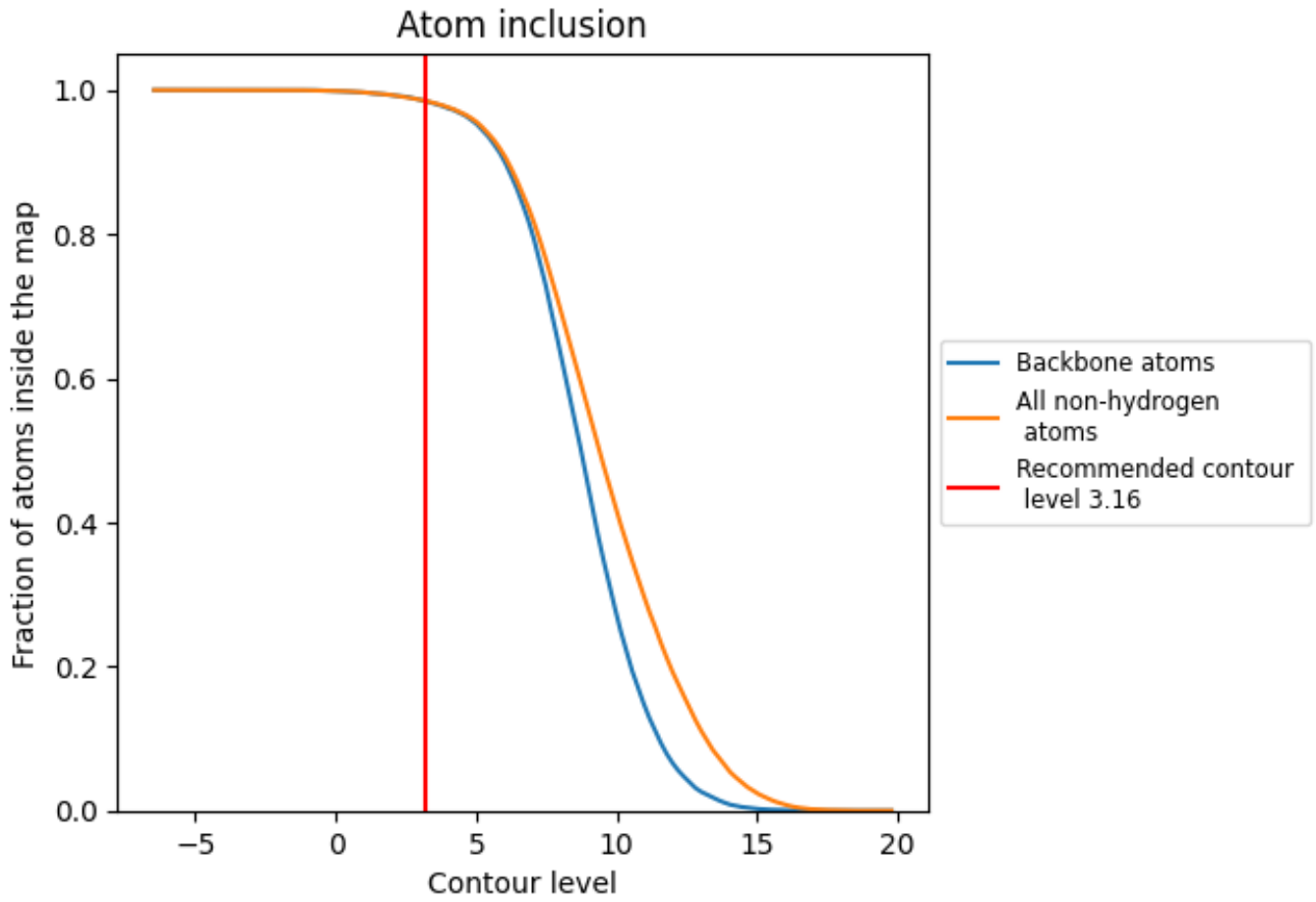
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.16).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 99% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (3.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9853	0.1530
A	0.9988	0.1730
B	0.9696	0.1270
C	0.9848	0.1370
D	0.9755	0.1140
E	0.9797	0.1420
F	0.9649	0.1330
G	0.8987	0.1010
H	0.9833	0.1310
I	0.9908	0.1110
J	0.9646	0.0940
K	0.9801	0.1120
L	0.9870	0.1060
M	0.9953	0.1390
N	0.9556	0.0920
O	0.9942	0.1460
P	0.9952	0.1050
Q	0.9731	0.1290
R	1.0000	0.1060
S	0.9968	0.1010
T	0.9985	0.1300
U	0.5602	0.0310
W	0.9350	0.1390